SUB- AND SUPER-CRITICAL EVAPORATION AND COMBUSTION OF A MOVING DROPLET

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SUMMARY: We are conducting a comprehensive computational study of fuel droplet evaporation and combustion in sub- and super-critical ambient conditions under forced convection. An experimentally validated model for a moving spherical droplet that undergoes evaporation has been developed. The model is used to predict droplet lifetimes and droplet penetration distances over a wide range of ambient pressures. In addition, a low pressure, experimentally validated model for a moving spherical droplet that undergoes combustion has been developed. This model employs a one-step overall reaction and is used to predict extinction velocities for different size droplets. Future work will allow for droplet deformation and semi-detailed chemical kinetics.

TECHNICAL DISCUSSION Two aspects of droplet evaporation/combustion have been studied and are discussed below.

I. Evaporation of a Spherical Moving Fuel Droplet over a Wide Range of Ambient Pressures within a Nitrogen Environment (with Dr. Hongtao Zhang). Modeling evaporation of moving fuel droplets within high pressure and high temperature environments is of critical importance in devices such as diesel engines, liquid-fueled rocket engines and high-output combustors for aircraft jet engines. Studies on droplet evaporation at elevated pressures have been mostly limited to stagnant surroundings.

In this study results have been obtained for evaporation of a n-heptane droplet translating within a high pressure and high temperature nitrogen environment. The axisymmetric numerical model that has been developed allows for inert species solubility in the liquid phase. Most studies on moving droplets assume a spherical shape. However, at a large Reynolds number, the Weber number may be large enough to cause deformation and even break-up of the droplet. The extensive numerical results of Dandy and Leal [1] show that the droplet remains nearly spherical for Weber numbers less than 1.0 even at Reynolds numbers as high as 400. We have employed the above criterion of droplet sphericity in our axisymmetric model to be consistent with our assumption that the droplet remains spherical. Future work at higher Weber numbers will allow for droplet deformation and possibly droplet break-up.

The gas and liquid phase solutions are obtained by solving the axisymmetric unsteady equations of mass, species, momentum, and energy conservation in spherical coordinates. These equations are coupled via the conservation equations at the interface and are solved iteratively. The effect of gravity is neglected. The finite-volume [2] and SIMPLEC [3] methods are used to discretize the governing equations in the computational domain. Staggered grids and the hybrid scheme are used in the discretization equations. Real gas effects are modeled using the Peng-Robinson equation of state with the appropriate binary interaction coefficient and transport and thermodynamic properties as recommended by Reid et al. [4]. Calculations are terminated when $(d/d_0)^2 \leq 0.2$, or when the critical state for the binary system is reached.

The current axisymmetric numerical model is validated by comparison to the experimental results of Gokalp et al. [5]. Fig. 1 presents the time histories of $(d/d_0)^2$ for n-heptane droplets with initial diameters of 1.43 mm (U_∞=2.53 m/s) and 1.18 mm (U_∞=6.00 m/s) evaporating in a nitrogen environment at an ambient temperature of 297 K and an ambient pressure of 0.101 MPa (1 atm) under micro-gravity conditions. The relative velocities between the droplet and the gas phase remain constant throughout the droplet lifetime. These conditions correspond to the experimental conditions in Gokalp et al. [5], with the exception that Gokalp et al. used air as the gas phase, whereas nitrogen is used in the current numerical model. The droplet lifetime can be obtained from Fig. 1. The droplet lifetimes from the experimental results of Gokalp et al. [5] and numerical results of Fig. 1 are listed in Table 1. Very good agreement is shown. The axisymmetric numerical model has been also validated using the n-heptane experimental data of Nomura et al. [6]. Extensive presentation can be found in Zhang [7].

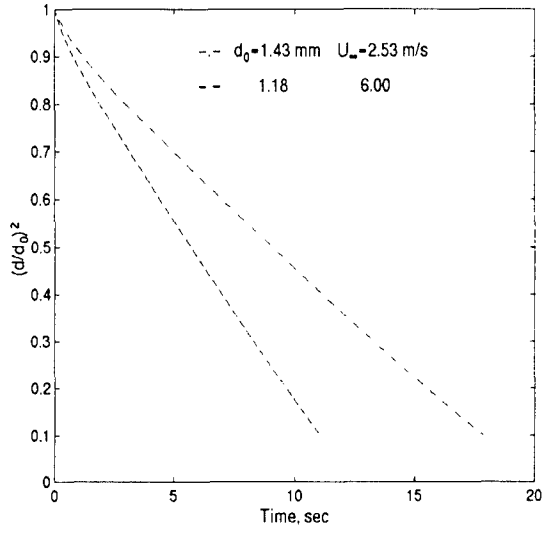


Table 1: Comparison of droplet lifetime

d_0 (mm)	U_∞ (m/s)	Lifetime (s)	
		Experimental [5]	Numerical
1.43	2.53	19.20	19.98
1.18	6.00	12.04	12.46

Fig. 1. Time histories of $(d/d_0)^2$ (p_∞ =0.101 MPa, T_∞ = 297 K)

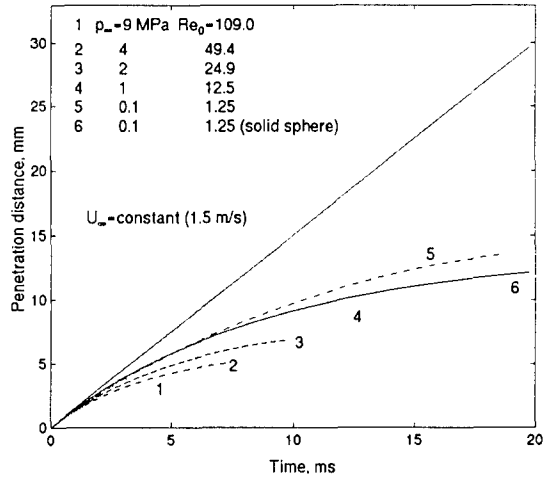


Fig. 2a. Droplet penetration distance with time for different ambient pressures ($U_{\infty 0}$ =1.5 m/s).

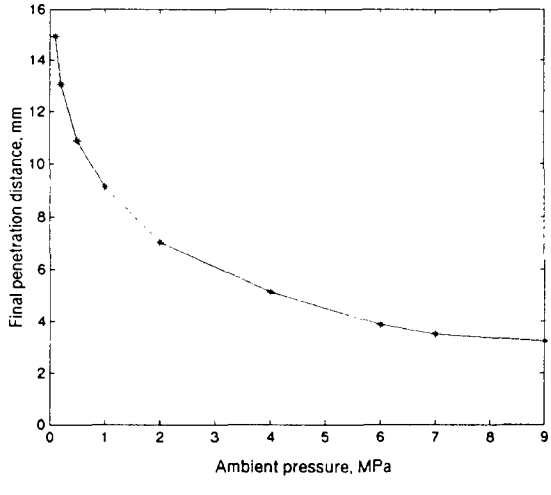


Fig. 2b. Final penetration distance with ambient pressures ($U_{\infty 0}$ =1.5 m/s).

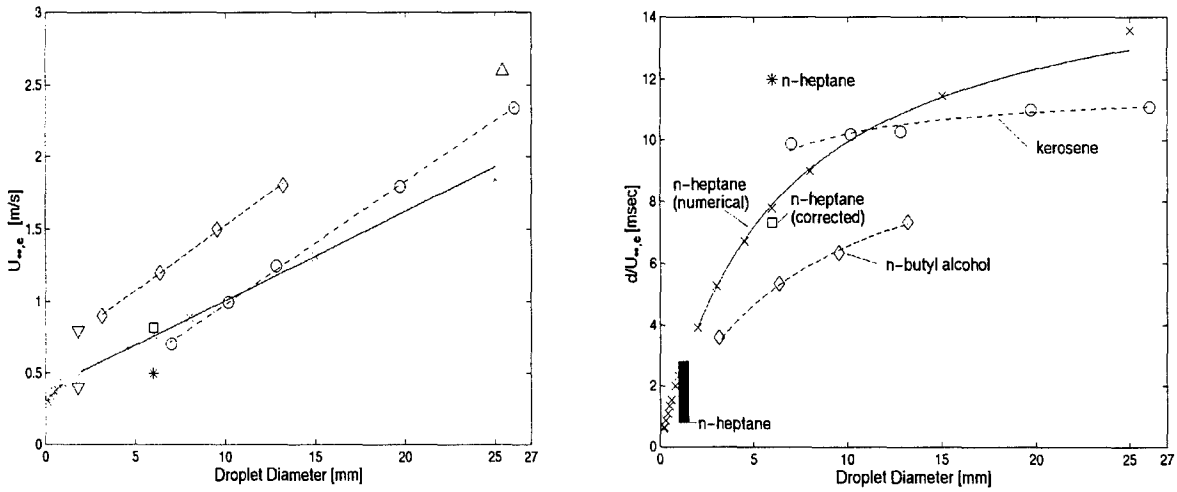
Results presented in Fig. 2 were calculated for a moving n-heptane droplet evaporating within a nitrogen environment. The initial diameter is 100 μm and the initial temperature is 300 K. Fig. 2a shows the droplet penetration distance as a function of time for different ambient pressures at an initial droplet velocity of 1.5 m/s. Cases 1-5 are for n-heptane droplets. The moving droplets experience deceleration while undergoing vigorous evaporation. The lower the ambient pressure, the larger the droplet penetration distance. Actually, the final droplet penetration distance decreases exponentially with ambient pressure (see Fig. 2b). In case 6, a solid sphere with the same density as in case 5 is considered, which is moving under the same ambient conditions (temperature and pressure) as in case 5. The drag coefficient for a solid sphere recommended by Mills [8] is employed. The reduction

in the drag force experienced by the evaporating droplet, a result known for a long time in the literature [9], leads to a higher droplet penetration distance (case 5) compared to that for the solid sphere (case 6). The straight solid line in Fig. 2a corresponds to the penetration distance of a solid sphere moving with a constant velocity.

II. Numerical Simulation of Droplet Extinction Due to Forced Convection (with doctoral student Daniel N. Pope).

The literature has shown that envelope flames surrounding droplets could extinguish in the presence of "adequately strong" convective flows. The present work numerically investigates the extinction of fuel droplets due to forced convection. A zero-gravity environment at atmospheric pressure is considered. The gas phase solution was obtained using the axisymmetric quasi-steady equations of mass, species, momentum, and energy conservation in spherical coordinates. Droplet internal circulation was accounted for by solving the quasi-steady momentum equations for the liquid phase. The gas and liquid phase were solved iteratively and coupled via the interfacial conservation equations. The governing equations were discretized using the finite volume [2] and SIMPLEC [3] methods. A staggered grid was adopted and relaxation was incorporated via an artificial time-step that was embedded in the discretization equations. Hyperbolic tangent stretching functions were used to concentrate grid points near the fore and aft lines of symmetry and at the droplet surface in both the gas and liquid phase. The discretization equations were solved using the ADI method with the TDMA used on each line of the two alternating directions.

A one-step overall reaction was used to describe combustion. Values for the activation energy, and oxygen and fuel concentration exponents in the finite-rate kinetics were adopted from Westbrook and Dryer [10]. The pre-exponential factor was determined by comparison of numerical results with experimental data [11] for extinction velocity. For n-heptane, a pre-exponential factor three times that of Westbrook and Dryer [10] was selected. An initial condition of a chemically frozen environment with a high temperature region near the droplet was used to cause ignition of the fuel/air mixture in the gas phase. The extinction velocity was obtained by selecting an initial freestream velocity that resulted in an envelope flame and then incrementing the freestream velocity by 1 cm/s between successive quasi-steady solutions until the evaporation constant exhibited a sharp decrease.



a: Extinction velocity vs droplet diameter

b: Flow time at extinction vs droplet diameter

Fig. 3. Extinction velocity and flow time vs. droplet diameter: (x) - numerical predictions for n-heptane under zero-gravity (T_∞= 300 K and p_∞= 1 atm). Experimental data under normal-gravity for various fuels in air at "room" temperature and atmospheric pressure; (o) - kerosene (Spalding [12]), (◊) - n-butyl alcohol (Agoston et al. [13]), (*) - n-heptane (Gollahalli and Brzustowski [15]), (□) - previous point corrected for natural convection, (∇) - gasoline (Agafonova et al. [16], lower: aiding natural convection, upper: opposing natural convection), (Δ) - n-heptane (Gore et al. [17]), (shaded box) – n-heptane (Chauveau et al. [18]).

Results are presented for extinction velocities of n-heptane droplets burning in air at room temperature (300 K) and a pressure of 1 atm. Droplet diameter (d) is varied from 0.18 to 25.0 mm to determine its effect on extinction velocity ($U_{\infty,e}$). The fact that the available experimental data for extinction velocities under microgravity conditions are very limited complicates the process of model validation. However, experimental data for the extinction velocities of various fuels under normal-gravity exist in the literature. These data have been very useful for a qualitative validation of our code. Fig. 3a shows the predicted extinction velocity for n-heptane droplets in air as a

function of droplet diameter. The value of $U_{\infty,e}$ = 0.43 m/s for d=1 mm corresponds to the results of Okajima and Kumagai [11]. This experimental study was used to determine the pre-exponential factor for our numerical model. The figure also includes experimental results from the literature for the extinction velocity of various fuels under normal-gravity. Spalding [12] and Agoston et al. [13] conducted porous sphere experiments employing kerosene and n-butyl alcohol, respectively. Both studies show that the extinction velocity varies linearly with diameter. Our numerical results (solid line) predict this linear dependence for approximately d > 2 mm. Large activation temperature asymptotics [14] also predict this linear dependence. The magnitudes of the measured extinction velocities in [12] and [13], however, differ from our predictions possibly because the fuels are different. Buoyancy effects are negligible for the size of porous spheres employed by Spalding [12] and Agoston et al. [13] due to the small Richardson number (~ 0.05). Gollahalli and Brzustowski [15] employed the same fuel (n-heptane) as we did in our simulations. The buoyancy-induced flow in their experiment aids the forced convection flow. Fig. 3a shows that the extinction velocity corrected for the presence of natural convection lies very close to the numerical prediction for the same fuel. In addition, Fig. 3a shows that for diameters in the range of 180 μm – 1000 μm, our numerical model predicts that the extinction velocity exhibits a nonlinear dependence. Extrapolating the linear curve predicted for larger droplets may provide an erroneous value for extinction velocities of droplets of, say, 100 μm, which are encountered in a typical spray.

The characteristic flow time at extinction ($d/U_{\infty,e}$) as a function of droplet diameter is shown in Fig. 3b. Spalding [12] observed a nearly constant flow time in his experiments using kerosene. This is to be expected since extinction velocity varies linearly with diameter, intercepts the vertical axis at a small velocity, and only extinction velocities for large diameters are reported. The numerically predicted flow time for n-heptane approaches a constant at much larger diameters and decreases rapidly with decreasing diameter. Additional experimental data for n-heptane from Chauveau et al. [18] for suspended droplets under normal-gravity conditions and diameters between 1.0 and 1.5 mm are shown in Fig. 3b (shaded box).

The numerical predictions are in good agreement with experimental results from the literature, despite the use of a one-step overall reaction. Extensive presentation of this study can be found in Pope [19]. Future modifications to the numerical code will include semi-detailed chemical kinetics.

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